Supporting Information

Mechanistic insights into an enantioselective synthetic strategy for 1,3-disubstituted planar chiral ferrocenes

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I. Comparison of energies of iron-containing species in low- or high- spin states

Table S1. Comparison of the calculated free energies of several important iron-containing species in different spin states. All calculations were performed at the PBE0-D3(BJ)/def2-TZVP-SMD//PBE0-D3(BJ)/def2-SVP-gas level of theory. Calculated energies at low spin (spin=1) were used as the relative zero-point energy for all species. The energies are all in kcal/mol.

	5	**10**	**12**	**15**	**23**
spin=1	0.0	0.0	0.0	0.0	0.0
spin=3	18.6	25.6	11.4	18.4	13.8
spin=5	118.8	3.1	25.3	36.5	0.7

II. NPA charge analysis for **ts7** and **ts7R**

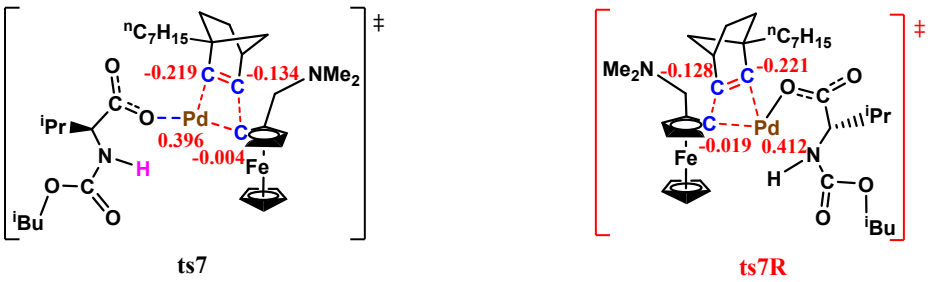

Fig. S1 NPA charge analysis for **ts7** and **ts7R** (a.u.).

III. NCI analysis for **ts7** and **ts7R**

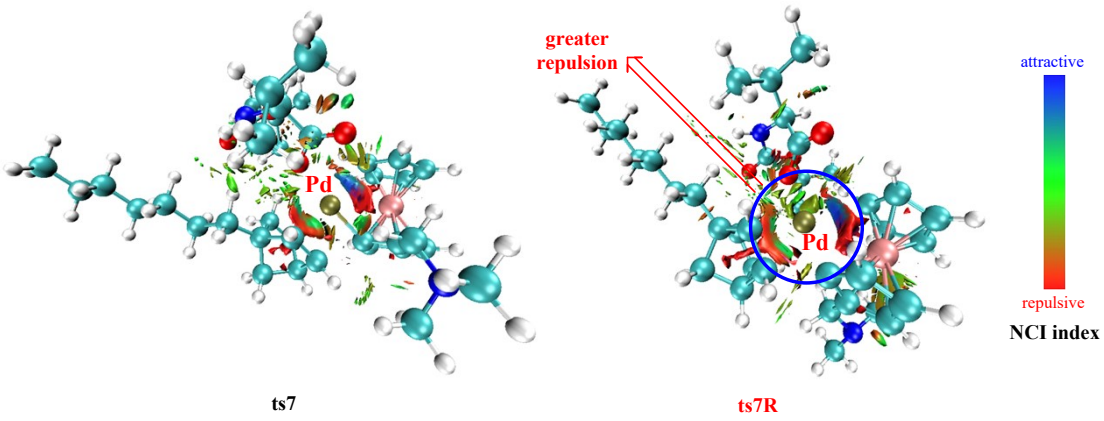

Fig. S2 NCI analysis for **ts7** and **ts7R**.